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Update on Interface Reconstruction and Related Topics in NIF ALE-AMR

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Livermore, CA, United States
June 2, 2008 through June 4, 2008

3rd International Workshop on High-Powered Laser Chamber Issues

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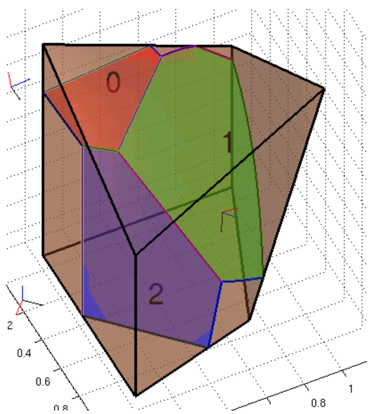
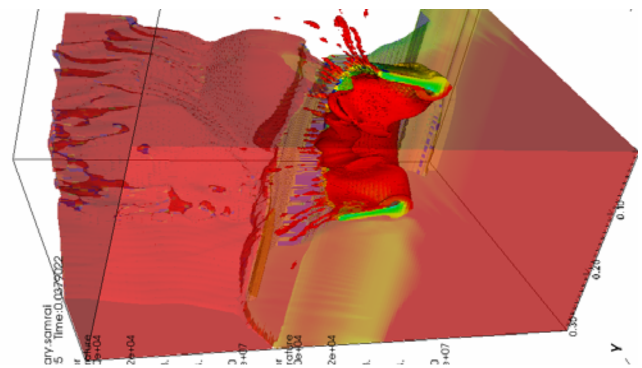
Update on Interface Reconstruction and Related Topics in NIF ALE-AMR





Nathan D. Masters

Contributors: Robert Anderson, Noah Elliot, Aaron Fisher, Brian Gunney, Tom Kaiser, Alice Koniges

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Basic steps of NIF ALE-AMR

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Initial Configuration

Lagrange Deformation

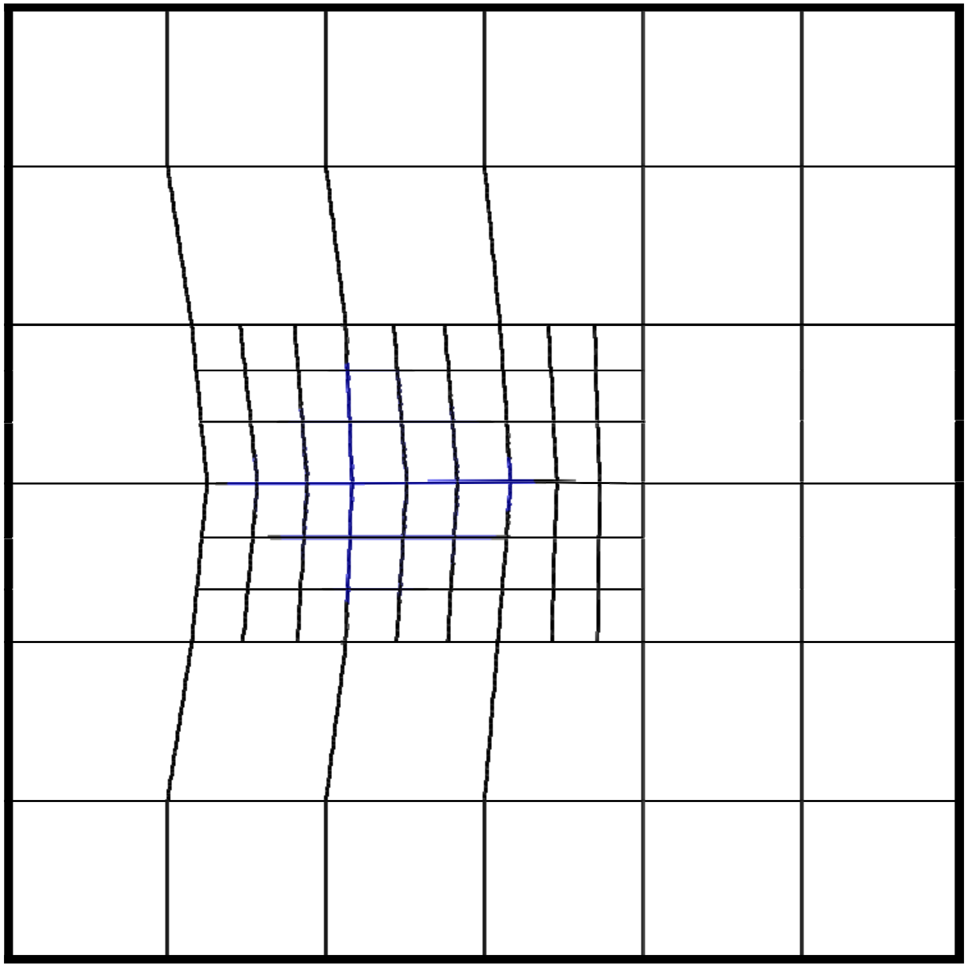
Mesh Relaxation

Advection

Remapped

Reconstruction

Coarsening/Refinement



NIF ALE-AMR represents material interfaces with a Volume of Fluid method

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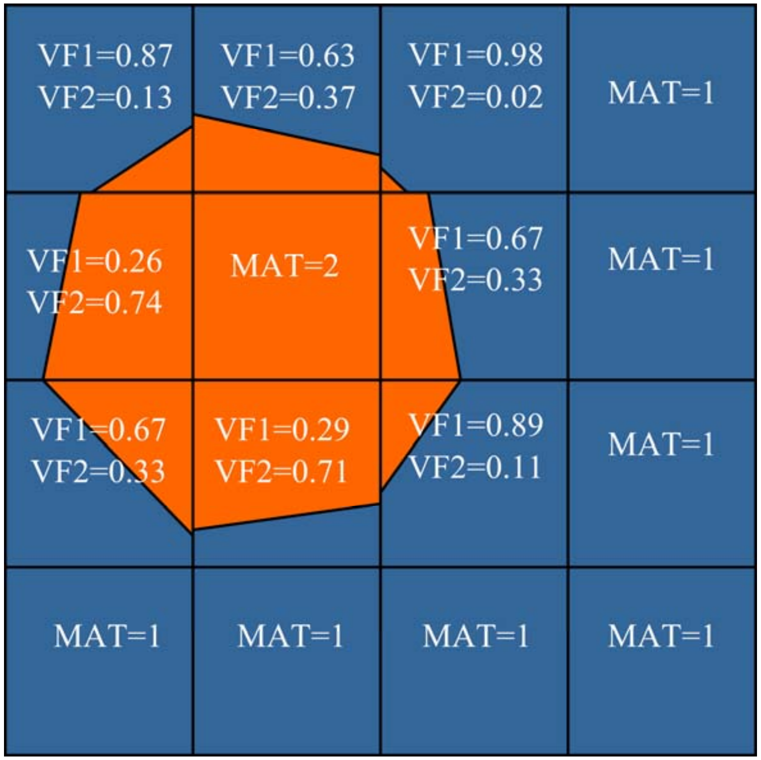
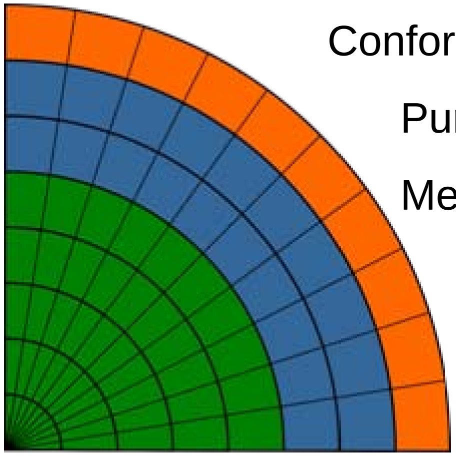
Volume of Fluid (VoF) uses volume fractions to reconstruct material interfaces when necessary



Alternative Methods



Conformal Mesh

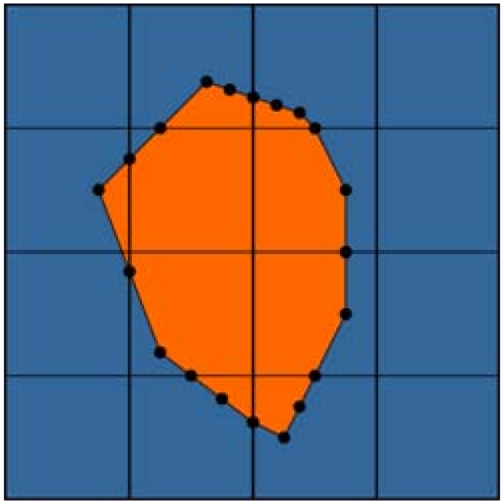
Pure Lagrangian

Mesh Entanglement

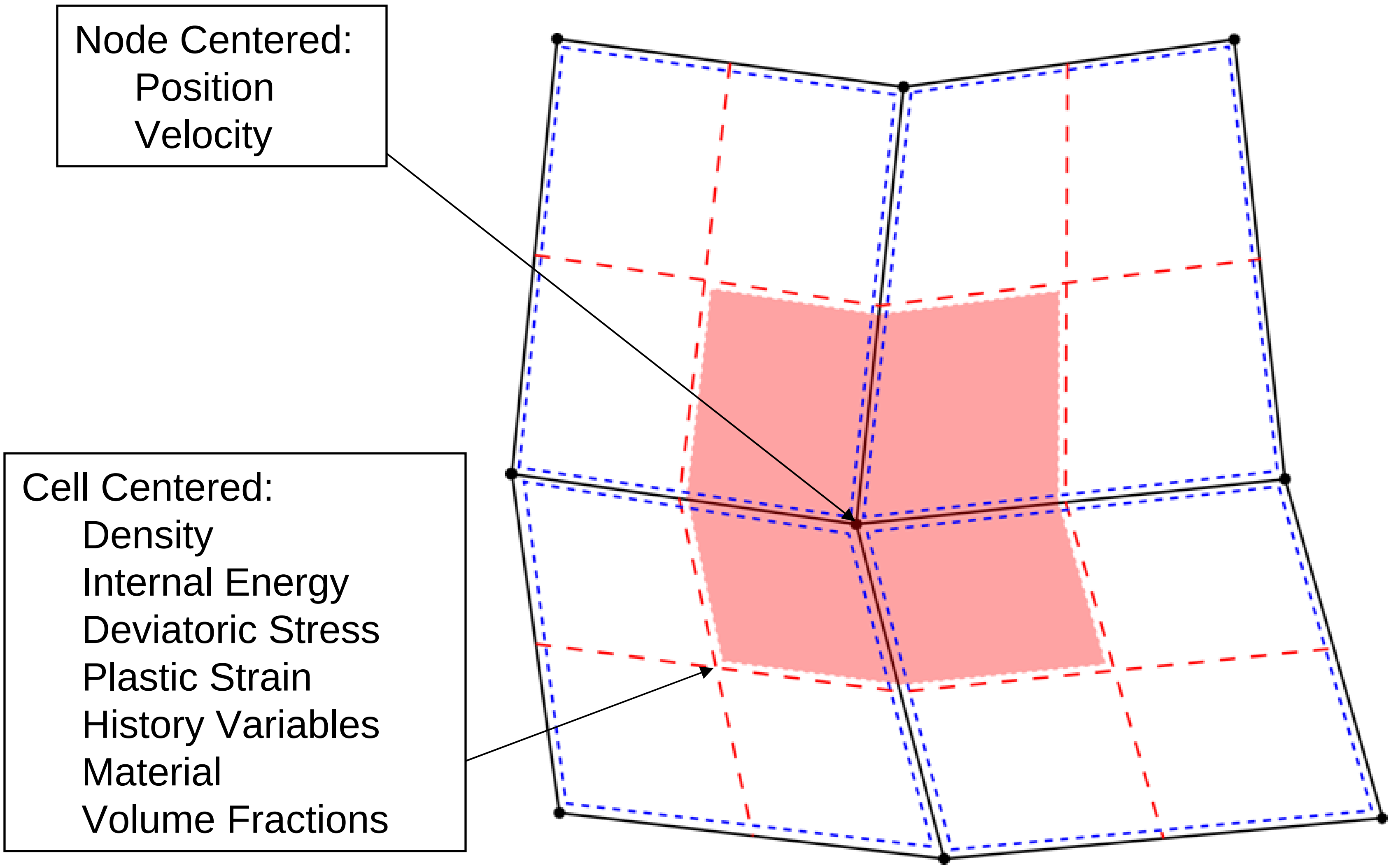
Tracking Particles

How many?

And where?



Staggered Mesh for Node- and Cell-centered quantities—cell centered quantities can be mixed



Most of the steps of NIF ALE-AMR are affected by Interface Reconstruction

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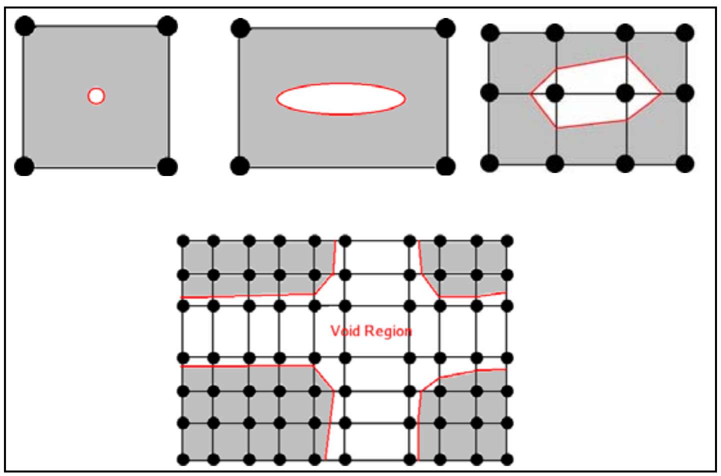
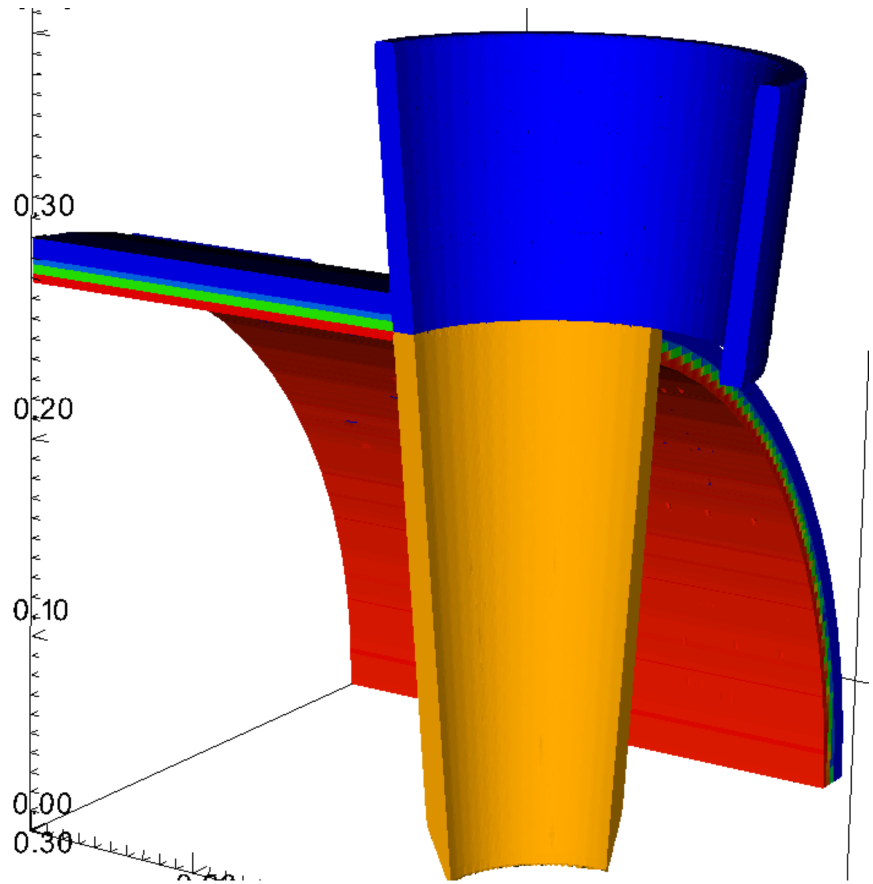
- Volume Fractions (VF) may set at startup by Shaping
- VF are modified during Lagrange Steps
  - Partitioning of strain
  - Insertion of void at fracture
- Advected during remapping
- Coarsened or Refined (AMR)



Fragmentation model depends on Interface Reconstruction for void formation, growth, coalescence and fracture



Shaping feature allows for meshing of complex structures without conforming to mesh boundaries.

Advection scheme avoids explicit reconstruction of the interface

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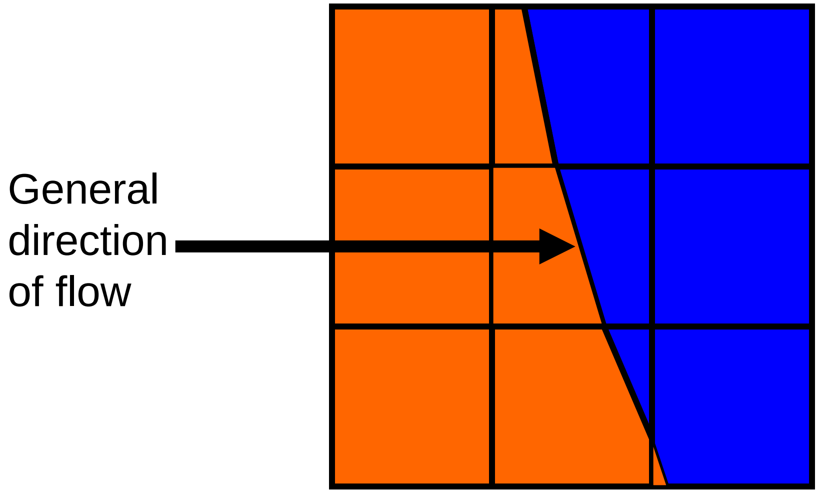
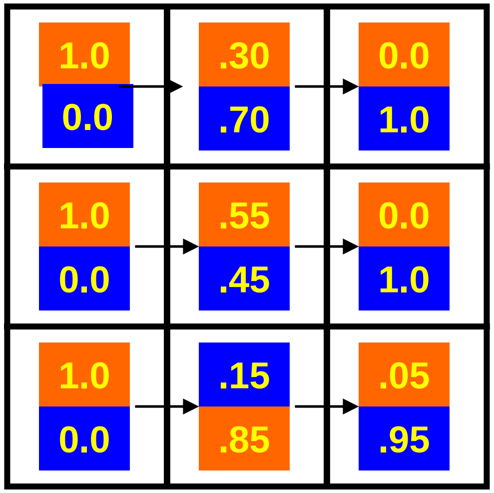
- In mixed material elements, interfaces between material components usually are not explicitly tracked
  - Only volume fractions are known
- How to determine material to transfer through volume fluxes?
- Estimate layout of materials in a zone by looking at volume fractions of materials in surrounding zones and direction of flux at each face



What's really happening



What the code sees

From Rob Neely, Salishan 2004, UCRL-PRES-203598

Algorithm determines the ordering and slopes of material interfaces during the advection step

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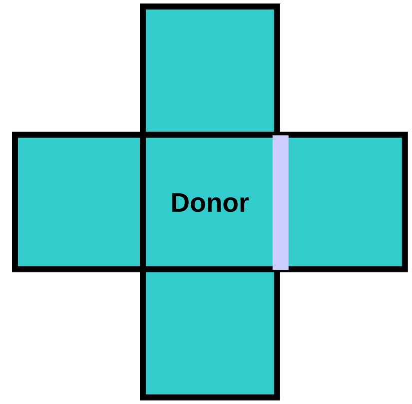
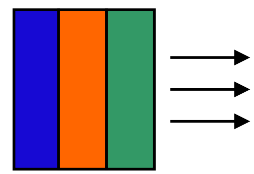
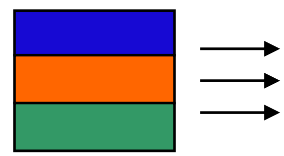
- CALE93 (Tipton) algorithm is one way to determine which materials will advect through a given volume flux
- A normalized slope is calculated at each face for each material in the upwind (donor) element.
- *Series* flow: Materials are moved in order in which they are stacked up relative to the face
- *Parallel* Flow: The components are moved simultaneously.
- *Corner* Flow: Treated as series flow until a critical volume fraction is achieved, at which point it becomes parallel flow.
- In the case where materials are advected simultaneously in all dimensions, care must be taken not to overdeplete the material in a zone
  - Three passes (leading/parallel ; middle ; trailing)
  - After each pass, material flux volumes must be rescaled



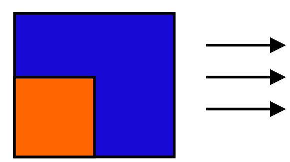
Slope at faces calculated from volume fractions in donor and its neighbors



Series



Parallel



Corner

From Rob Neely, Salishan 2004, UCRL-PRES-203598

But sometimes things (Advection) just don't work out the way you would like…so you fix them (Repair)

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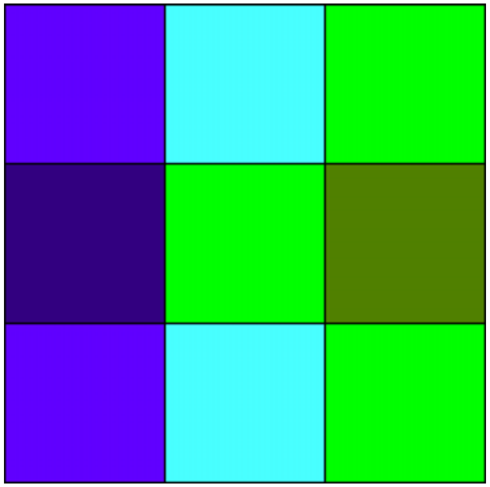
- In clean cells, the slopes at the faces are used to determine the advected quantities (density, internal energy, etc.)
- There is no general basis for such a slope in mixed zones so the the component materials of a mixed zone are assumed to have uniform properties.
- Roundoff Error in the Cleanout of Cells:
  - Large differences in material density
  - Small total mass and round off in the balance of momentum and momentum flux (or energy and energy flux) may result in large spurious velocities or energy

$$U^{(n+1)} = \frac{1}{m^{(n+1)}}\left((mU)^{(n)} + \sum_{i=1} \phi_i \right)$$

$$e^{(n+1)} = \frac{1}{m^{(n+1)}}\left((me)^{(n)} + \sum_{i=1} \phi_i \right)$$

- Solution: Repair this by borrowing quantities from neighboring zones in a conservative manner



Repaired state

- Repaired zones were effectively "broken," so the error introduced by Repair is worth being able to continue the simulation
- Floors and Ceilings are also used when necessary

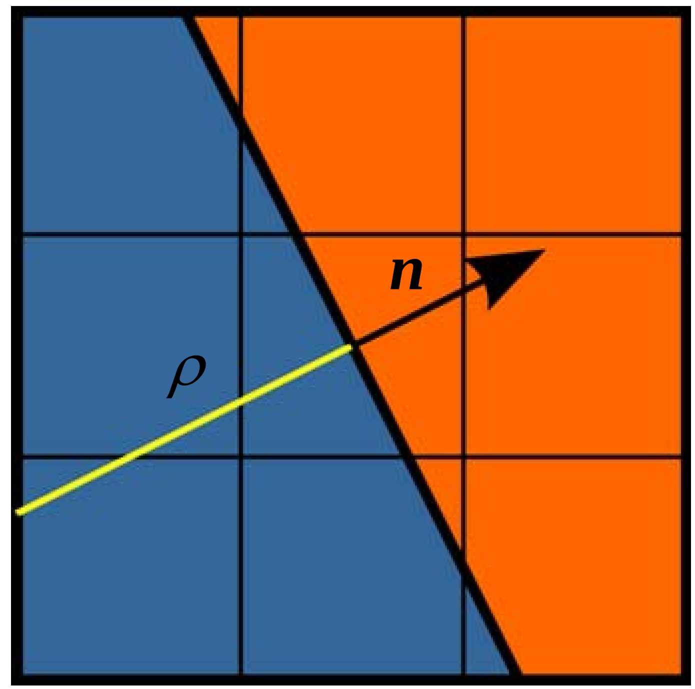
Shashkov and Wendroff, JCP, 198, 2004

AMR: Coarsening is easy, Refinement requires explicit interface reconstruction

- Sum of volume fractions

$$V_f^c = \sum_i V_{f,i}^f V_i^f \Big/ \sum_i V_i^f$$

- Orientation ($\boldsymbol{n}$) uses V_f's of neighboring cells
- Solve for location (ρ) of interface
- Assign refined V_f's



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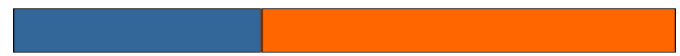
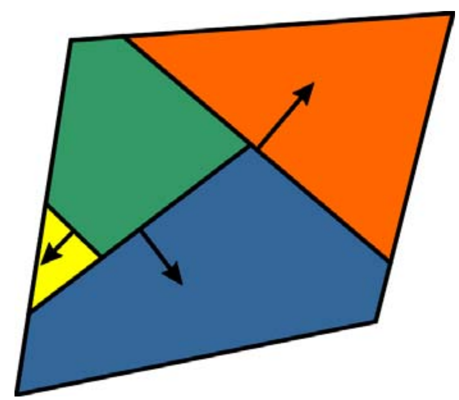
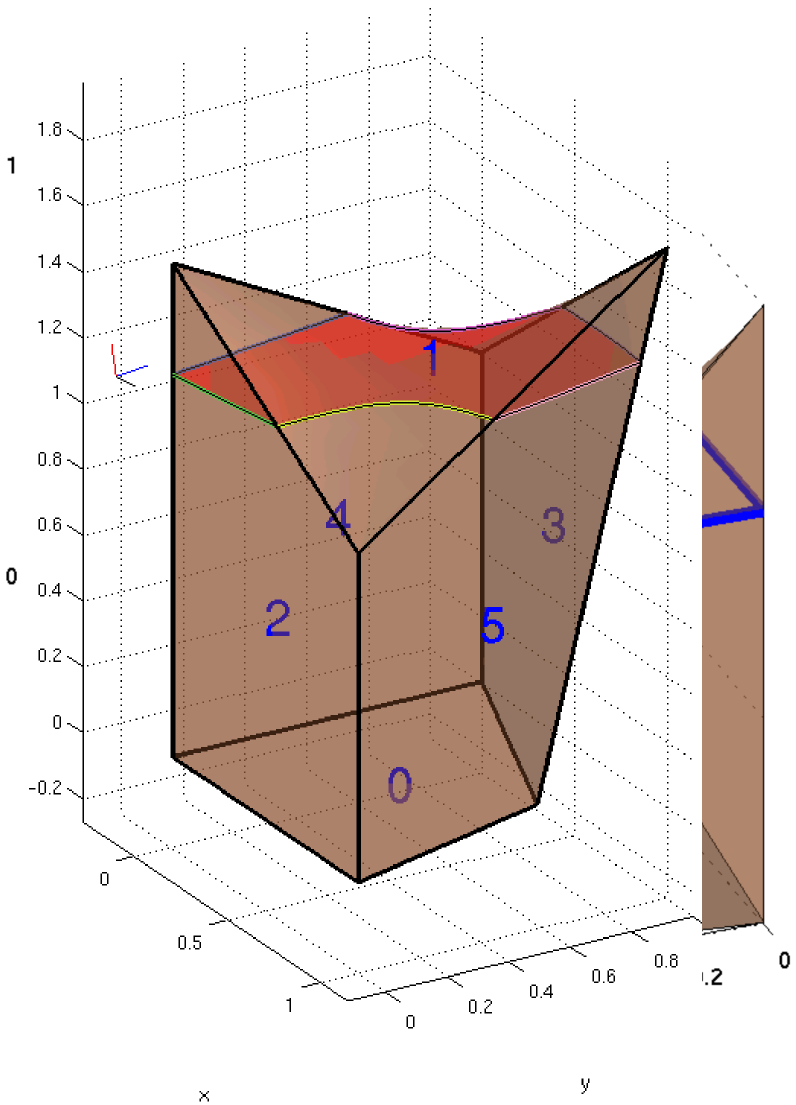
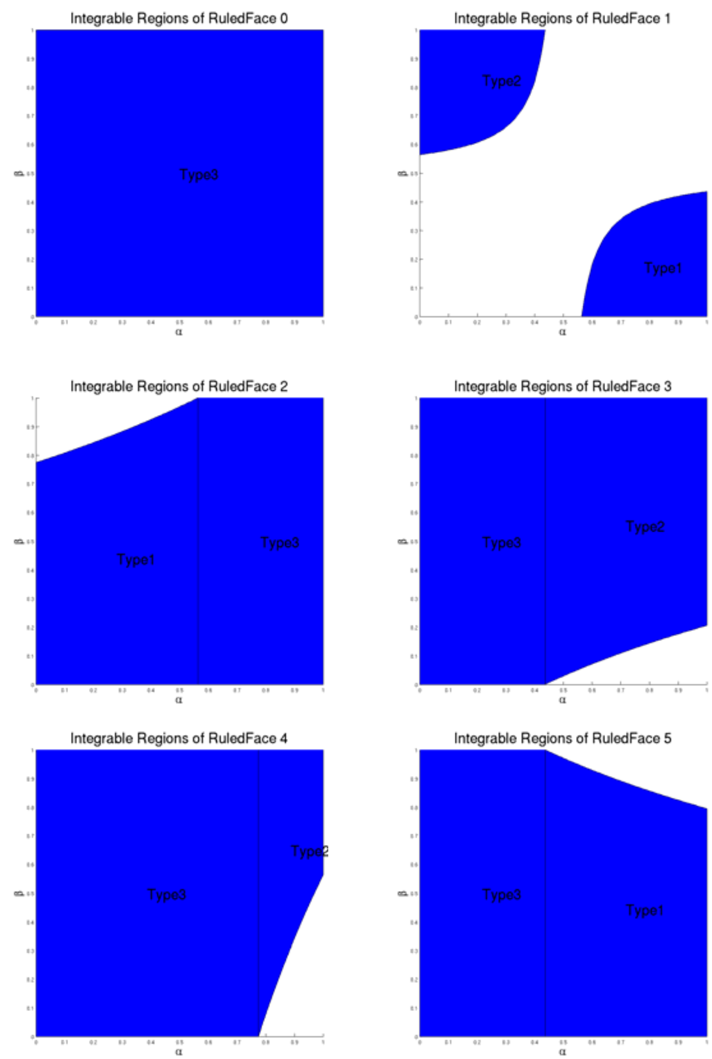
- 1D: 
- 2D: Polygons



- 3D: Truncated Hexahedra, bounded by doubly-ruled surfaces (DRS, or hyperbolic-paroboloids)

Intersections with DRS are hyperbolic in the intersecting plane and in the parametric space of the DRS (but may degenerate to parabolas, lines, or points)





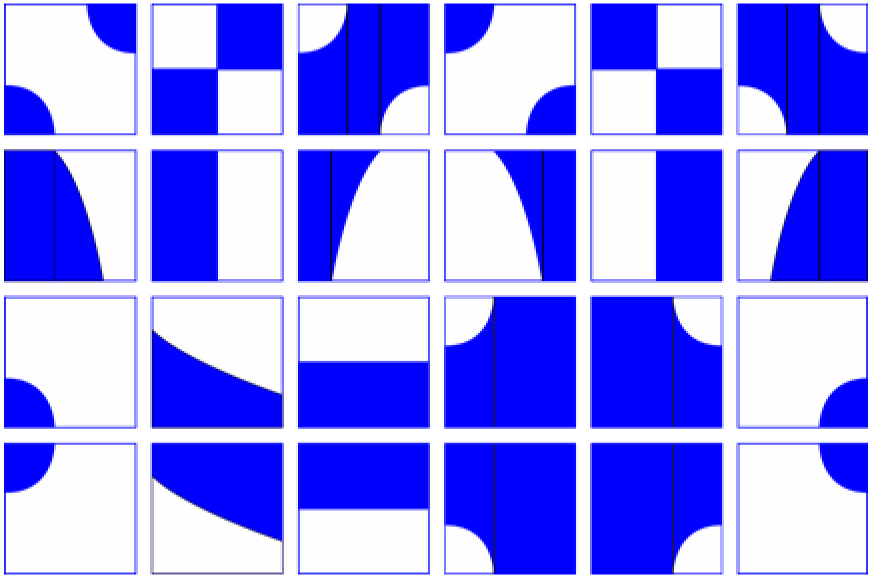
Volume contributions of truncated Doubly-Ruled Surfaces to the partial volume may be broken down in terms of integrable regions on the DRS

- Volume of Truncated Zone (for a single planar interface)

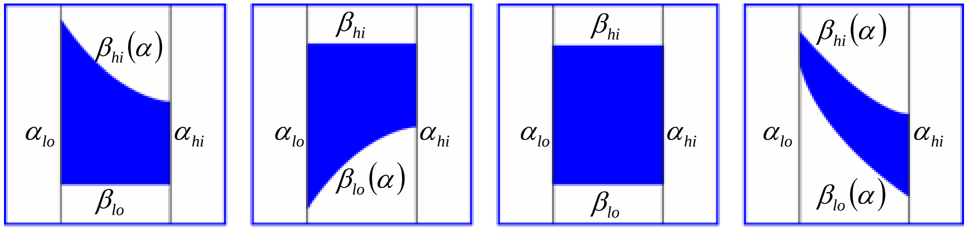
$$V_{tr} = \frac{1}{3}\left[\sum_{f=1}^{6}\int_{tr}(\boldsymbol{x}-\boldsymbol{n}\rho)\cdot \mathrm{d}\boldsymbol{S}_f(\boldsymbol{x}) + \int_{tr}(\boldsymbol{x}-\boldsymbol{n}\rho)\cdot \mathrm{d}\boldsymbol{S}_p(\boldsymbol{x})\right]$$

$$V_{tr} = \frac{1}{3}\sum_{f=1}^{6}\left\{(\boldsymbol{x}_1-\boldsymbol{n}\rho)\cdot\left[\boldsymbol{X}_1 K_{00} + (\boldsymbol{X}_3-\boldsymbol{X}_4)K_{10} + (\boldsymbol{X}_4-\boldsymbol{X}_1)K_{01}\right] - v_{tet}K_{11}\right\}$$

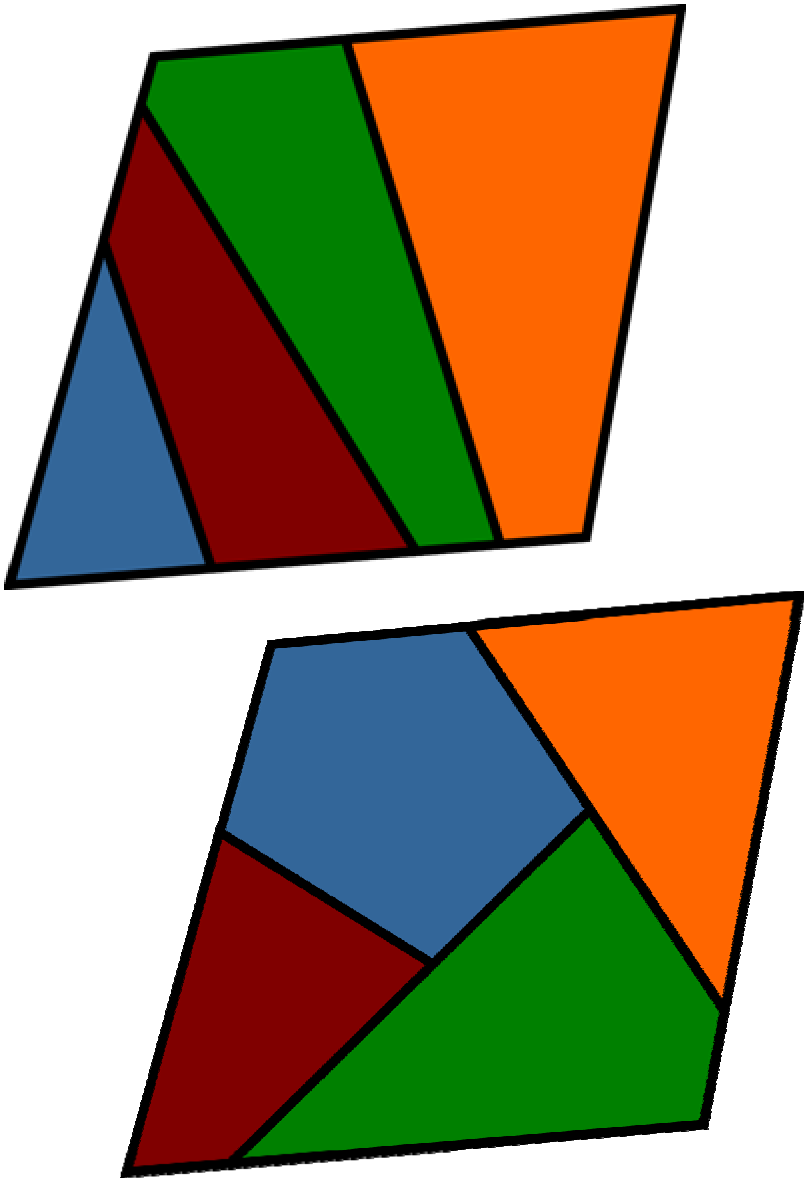
$$K_{nm} = \int_{\alpha_{lo}}^{\alpha_{hi}}\int_{\beta_{lo}(\alpha)}^{\beta_{hi}(\alpha)} \alpha^n \beta^m \,\mathrm{d}\beta\,\mathrm{d}\alpha$$

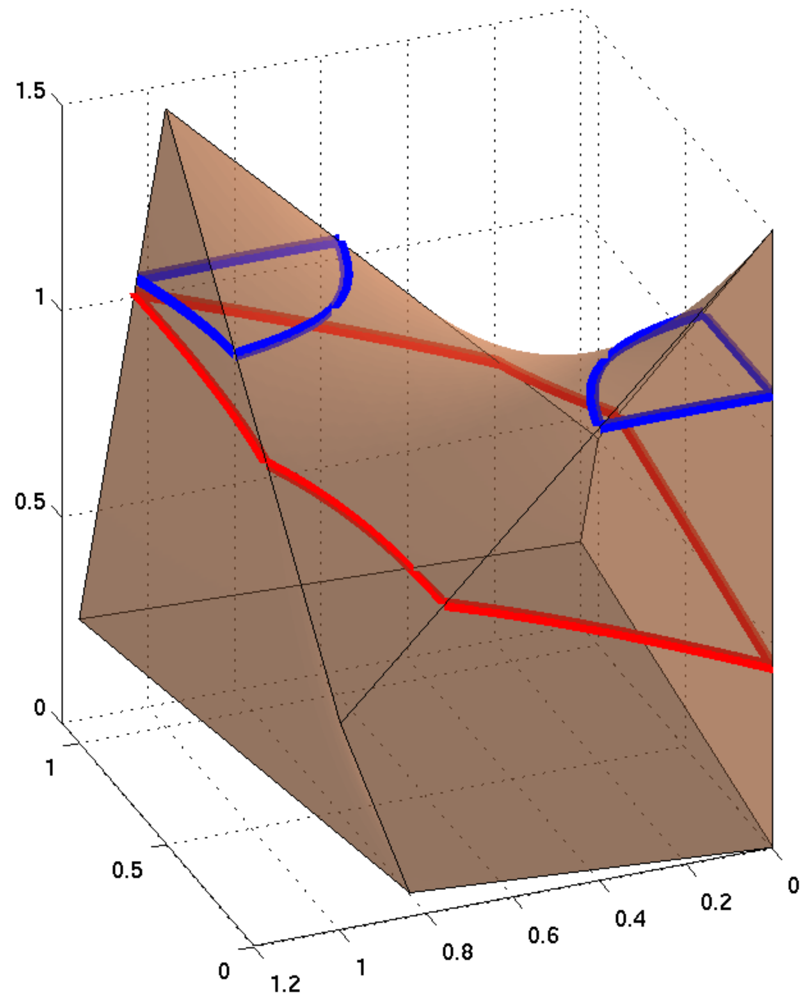


- 24 Classes of Intersections
- 4 Types of Integrable Regions
- All integrals in terms of logarithms and arithmetic operations
- K_{nm} terms remain constant



Multiple interfaces (materials) may result in onionskin and non-onionskin topologies





In 3D Non-onion skin topologies are treated by finding intersections of integrable regions…

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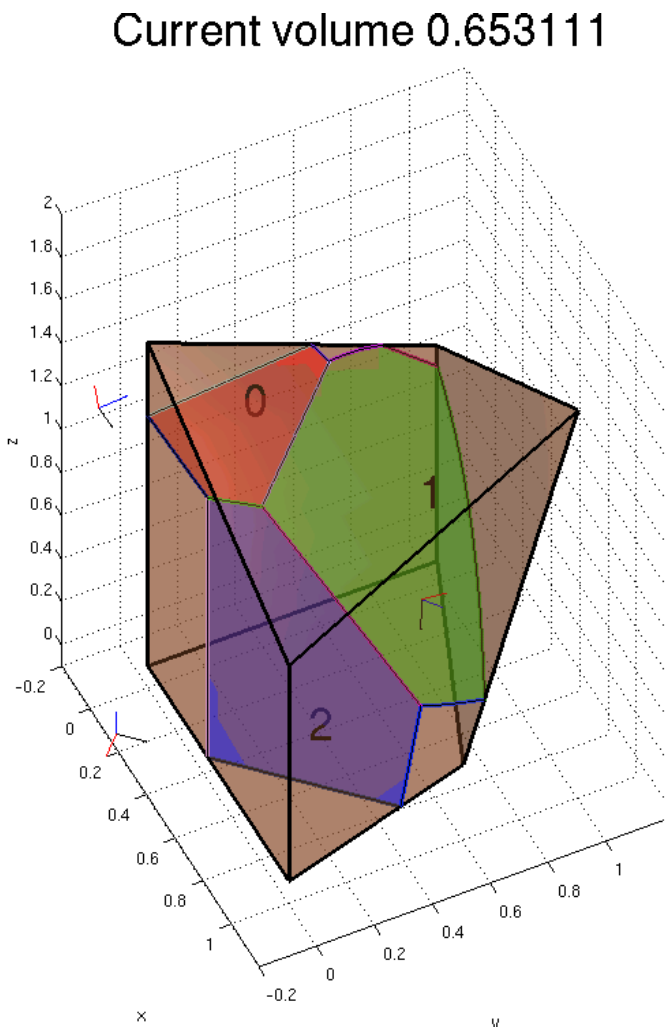

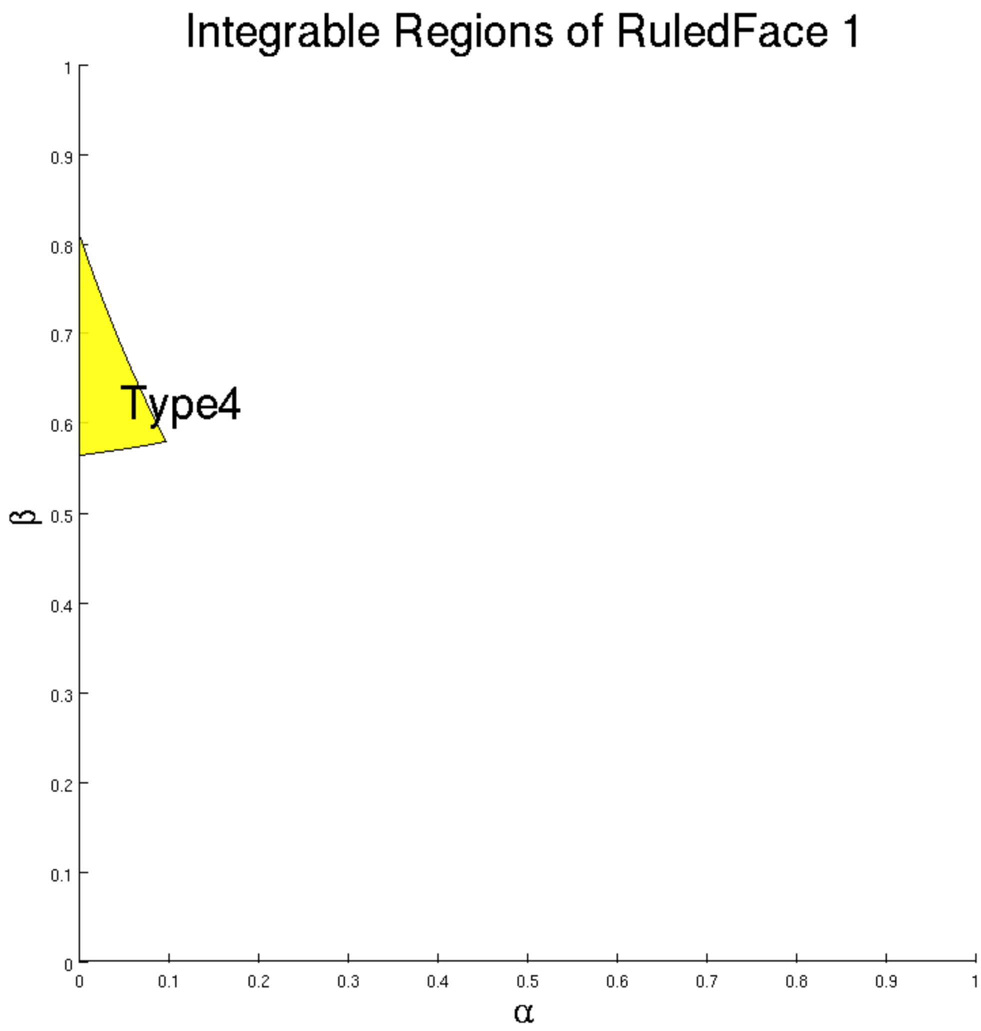

Similar to Vatti's polygon clipping algorithm (Vatti, *Comm. of ACM*, 1992)

Previous truncating planes may also contribute to the partial volume

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- Truncated volume equation

$$V_{tr}=\frac{1}{3}\left[\sum_{f=1}^{6}\int_{tr}(\boldsymbol{x}-\boldsymbol{n}\rho)\cdot\mathrm{d}\boldsymbol{S}_f(\boldsymbol{x})+\sum_{p=1}^{P-1}\int_{tr}(\boldsymbol{x}-\boldsymbol{n}\rho)\cdot\mathrm{d}\boldsymbol{S}_p(\boldsymbol{x})\right]$$

- Contribution of planar face expressed in terms of line integrals over the bounding contours (extracted from integrable regions and plane-plane intersections)

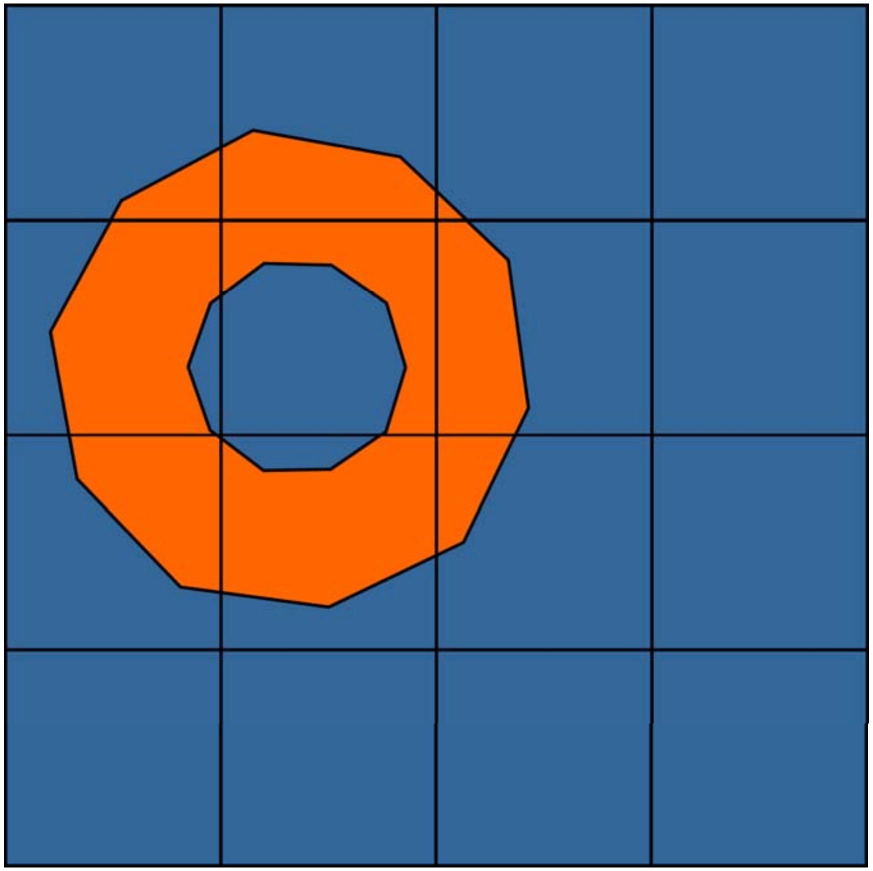
$$\begin{aligned}3V_p&=\int_{tr}(\boldsymbol{x}-\boldsymbol{n}\rho)\cdot\mathrm{d}\boldsymbol{S}_p(\boldsymbol{x})\\&=\frac{1}{2}(\rho'-\boldsymbol{n}\cdot\boldsymbol{n}'\rho)\sum_{j=1}^{contours}\int_{tr_j}\left(x_j'(\alpha)\frac{\mathrm{d}y_j'(\alpha)}{\mathrm{d}\alpha}-y_j'(\alpha)\frac{\mathrm{d}x_j'(\alpha)}{\mathrm{d}\alpha}\right)\mathrm{d}\alpha\\&=(\rho'-\boldsymbol{n}\cdot\boldsymbol{n}'\rho)A_p\end{aligned}$$

- Complete equation for non-onionskin topologies

$$V_{tr}=\frac{1}{3}\left[\sum_{f=1}^{6}\left\{(x_1-n\rho)\cdot\left(X_1\sum_{i=1}^{IR_f}K_{00,i}+(X_3-X_4)\sum_{i=1}^{IR_f}K_{10,i}+(X_4-X_1)\sum_{i=1}^{IR_f}K_{01,i}\right)-v_{tet}\sum_{i=1}^{IR_f}K_{11,i}\right\}+\sum_{p=1}^{P-1}\left\{(\rho_p'-n\cdot n_p'\rho)A_i\right\}\right]$$

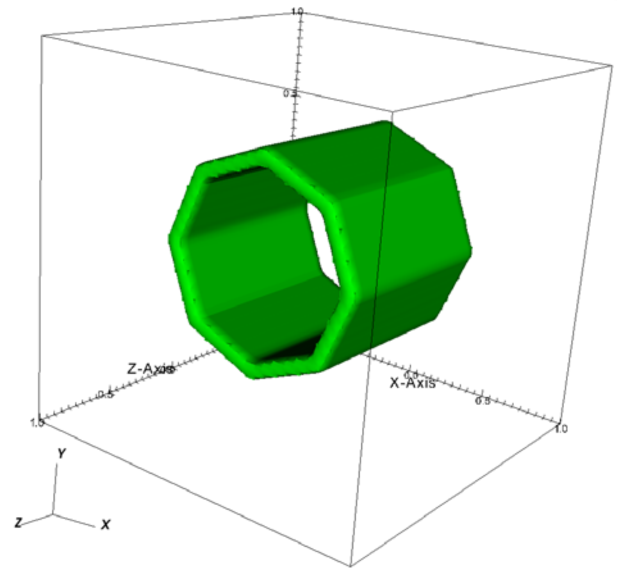
Interface reconstruction may also be used for shaping geometries: 2D Polygons

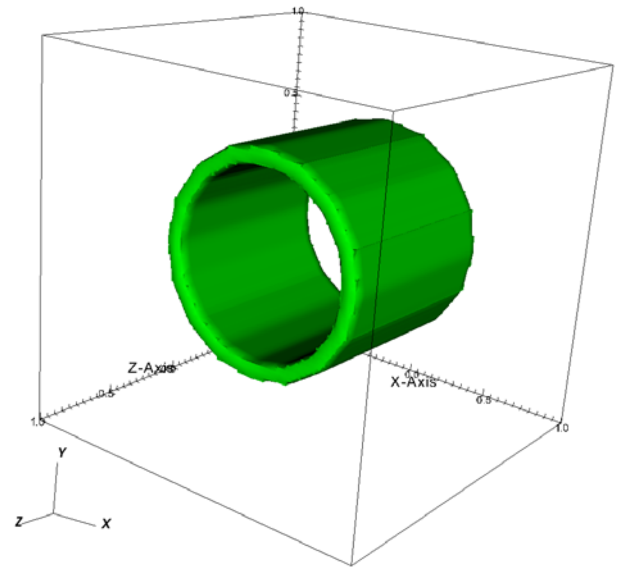
- In 2D shaping involves overlaying polygons on the mesh and evaluating the partial volumes
- Hollow geometries formed by shaping in with background material (air or void)



Shaping in 3D uses faceted surfaces

- Currently we have surfaces of revolution, but extrusions would be easy
- Current system uses minimum partial volume (Onionskin) Interface Reconstruction model
- Non-onionskin model is almost ready to take over shaping
- Shaping may also be used to set densities and internal energies within the same material





Aluminum cooling ring loaded with a radial impulse demonstrates fragment formation

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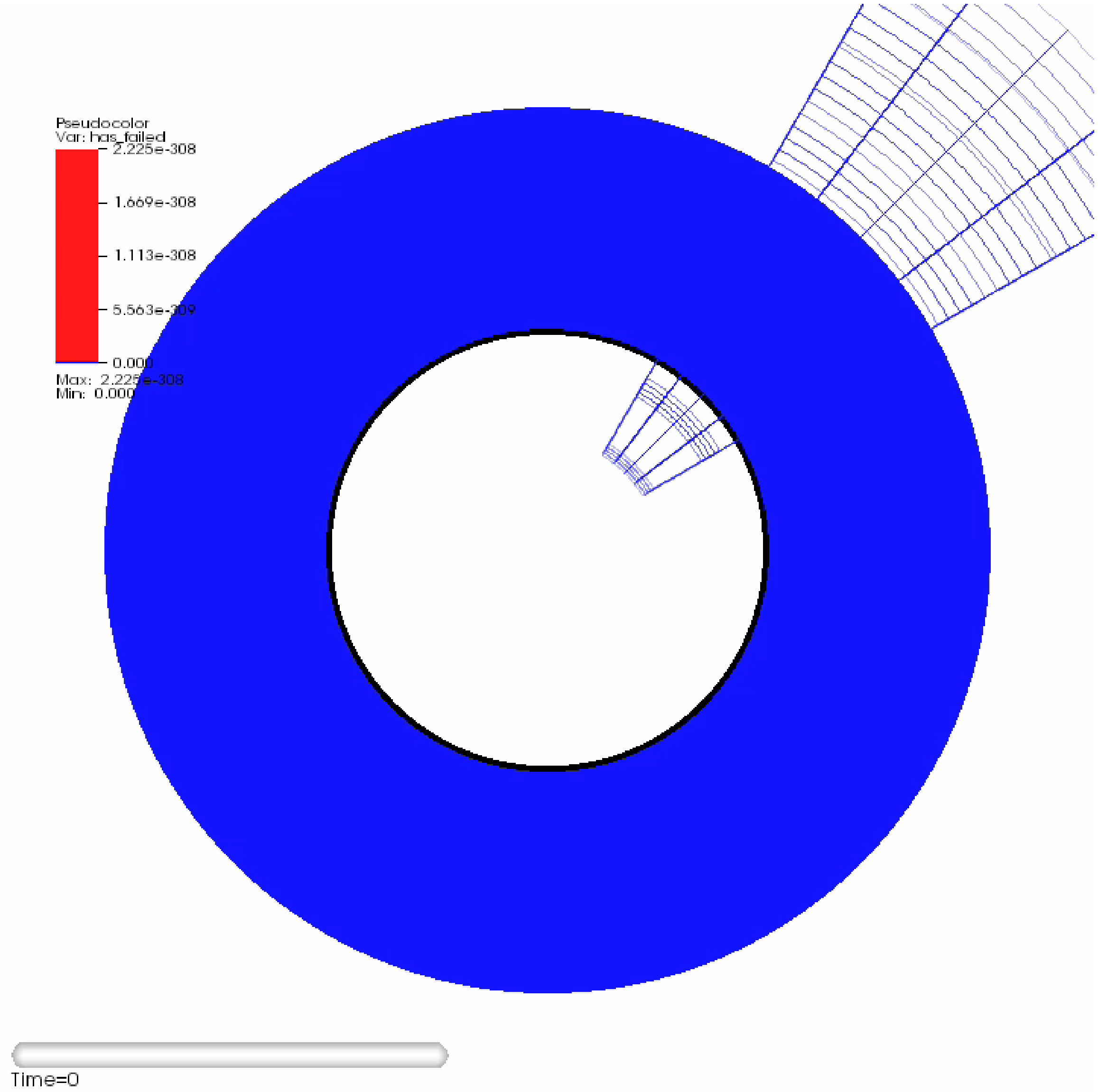

Copper cooling ring simulations predict notched ring may generate larger fragments

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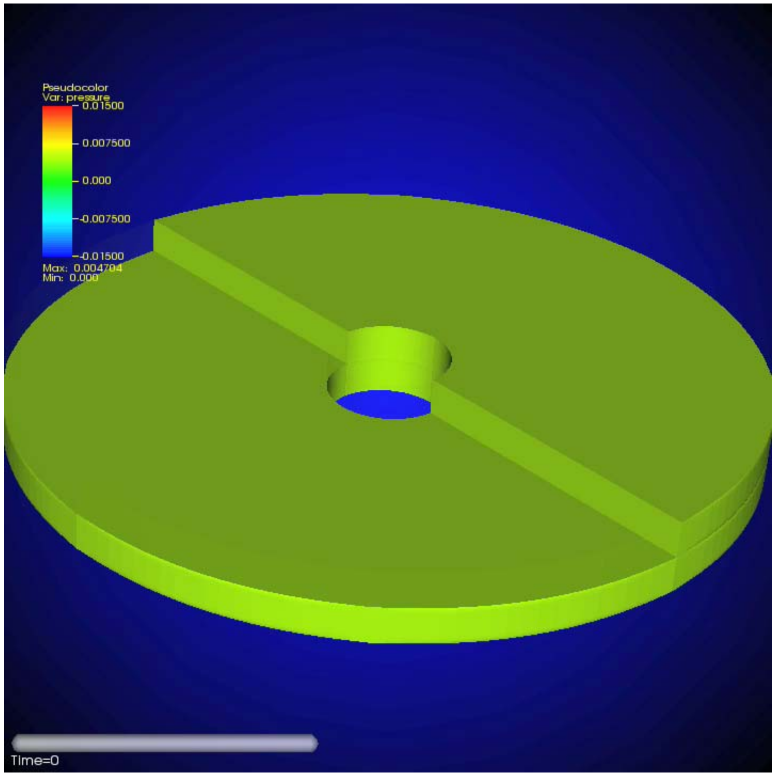

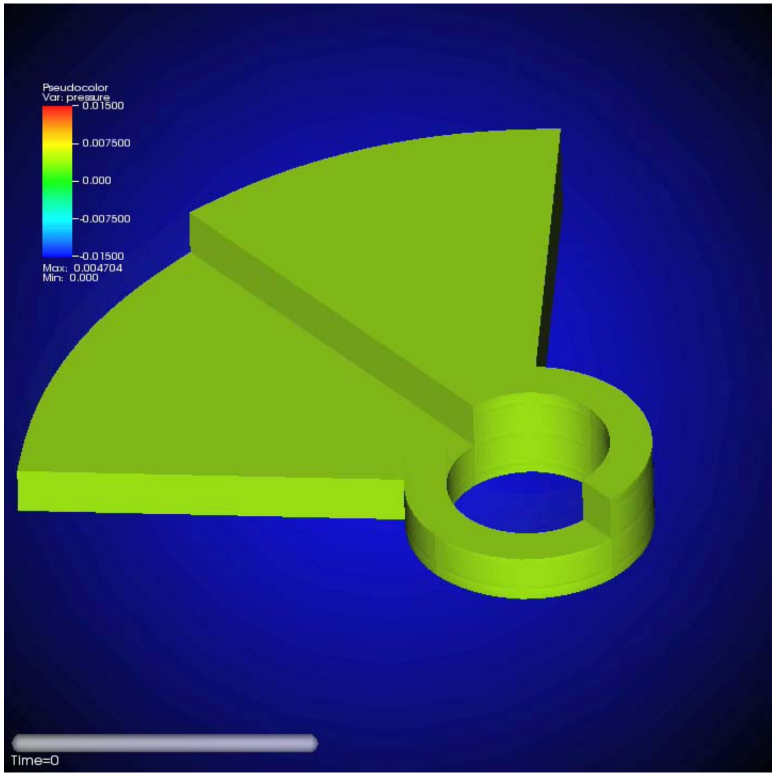

The keyhole diagnostic target allows VISAR access to the interior of the capsule

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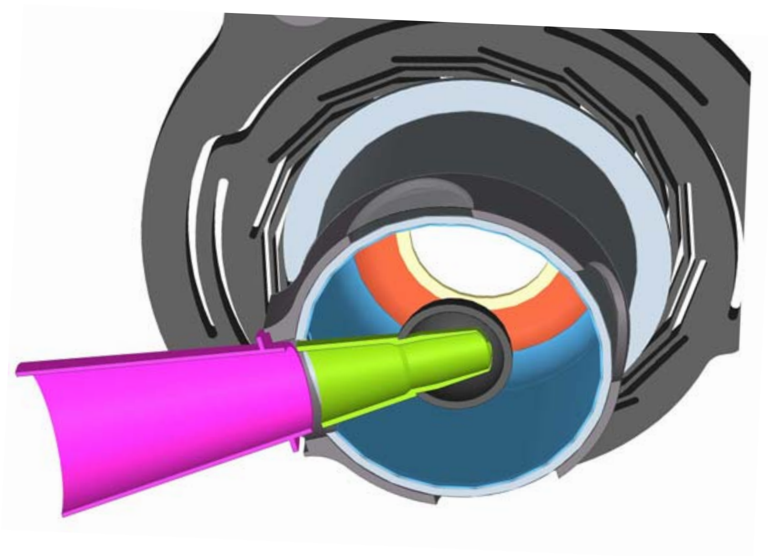
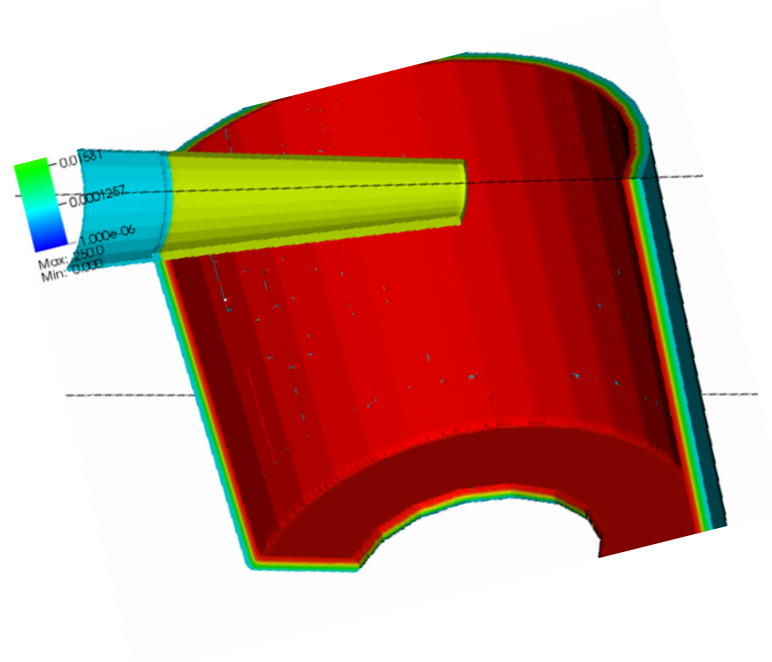
- Engineering drawing



- NIF ALE-AMR simulation geometry in an non-uniform Cartesian mesh



Surfaces of revolution used to shape geometry and initial conditions extracted from other simulations

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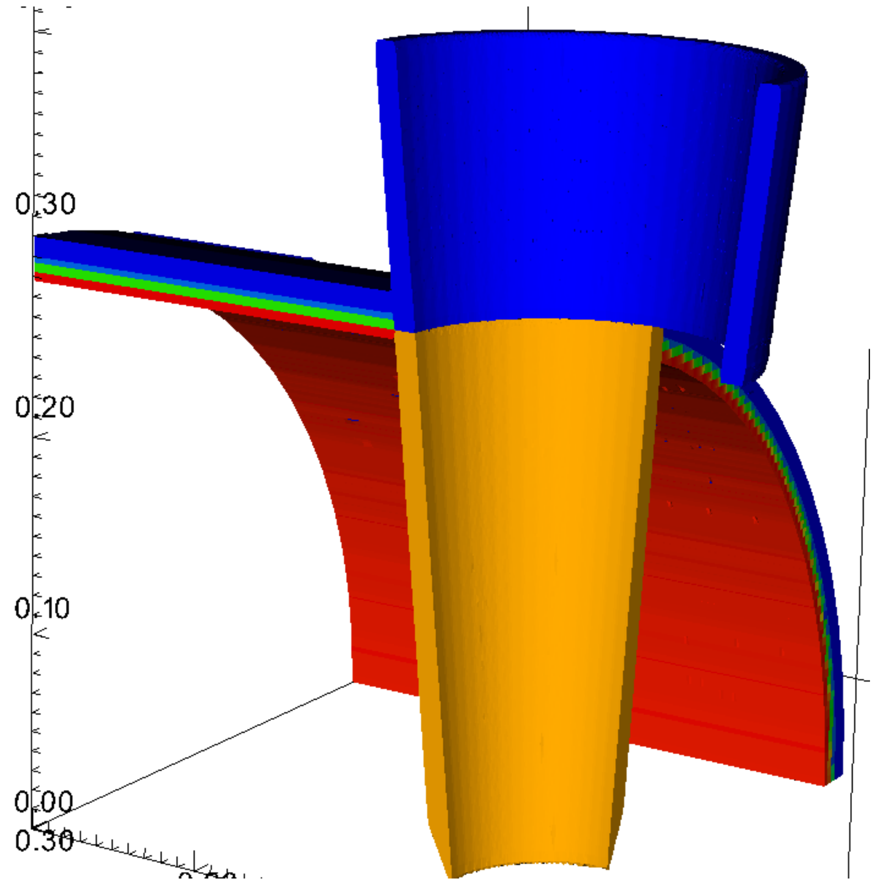
- Hohlraum (Modeled as Al)
  - Diameter 0.6 cm
  - Thickness 0.022 cm
- Energy Deposition
  - e=2.5e2 Mbar-cc/g, ρ=0.001 g/cc to depth of 0.004 cm
  - e=7.5e-1 Mbar-cc/g, ρ=5.0 g/cc to depth of 0.008 cm
  - e=1.5e-2 Mbar-cc/g, ρ=3.5 g/cc to depth of 0.012 cm
  - e=8.39e-5 Mbar-cc/g, ρ=2.7 g/cc remaining thickness
- Inner Cone
  - 2.5e1 ρ=2.7 g/cc 0.02 cm thick
- Outer Cone
  - 8.39e-5 D=2.7g/cc 0.02 cm thick (alternate design steps down to 0.01 cm)



Velocity of outer cone is small (good) but shape charge plume from inner cone material warrants further study

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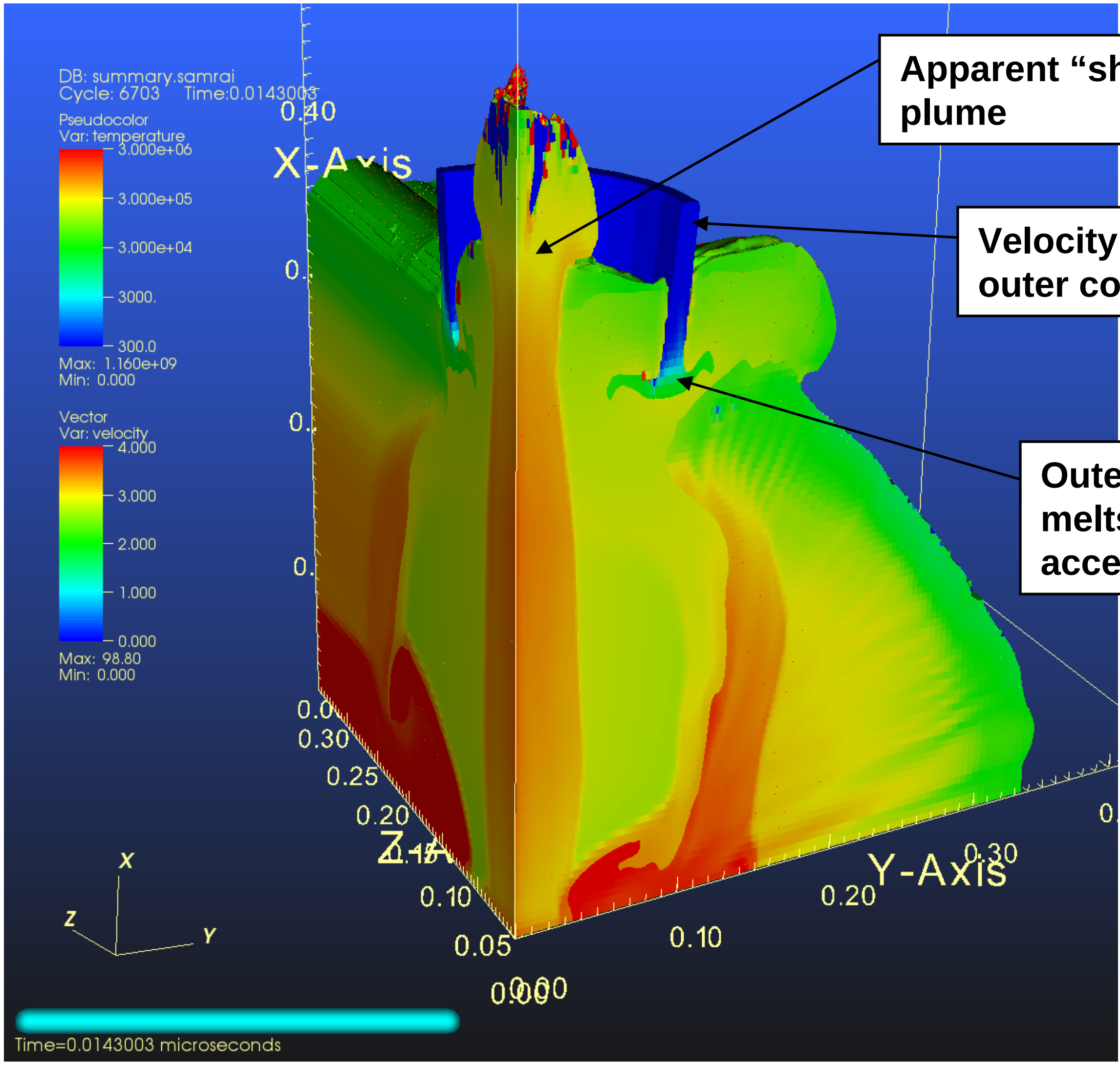

Apparent "shaped charge" plume

Velocity of remaining solid outer cone is negligible

Outer cone melts/vaporizes as it accelerates.

Keyhole simulation has driven a number of important developments:

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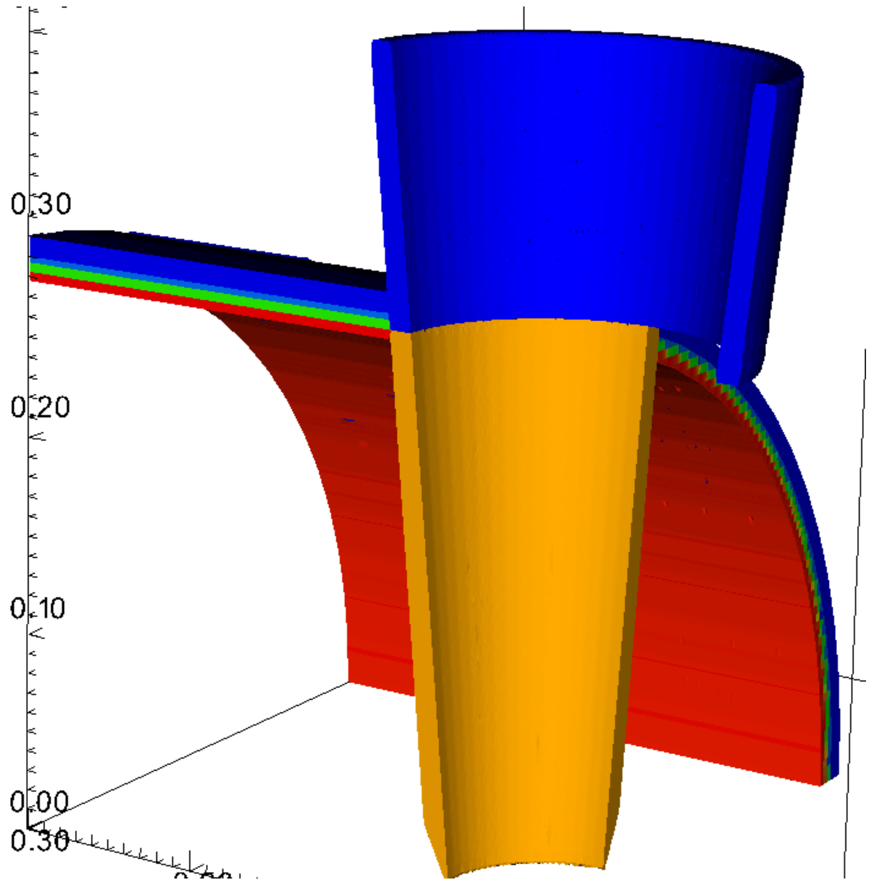
- Surfaces of Revolution
- Reworked internal storage for mixed quantities for more efficient insertion of data
- Introduced Melt to remove unnecessary data associated with strength
  - Saves 20 floating point values per melted region
  - Retains EOS
  - Ability to visualize solid/liquid and solid-vapor interfaces
- Reworked Repair
- Application of floors and ceilings to velocities, density, and internal energy
- Added ability to plot mixed state variables for improved visualization
  - States of mixed components may be inspected



Laser raytracing is currently being added to NIF ALE-AMR

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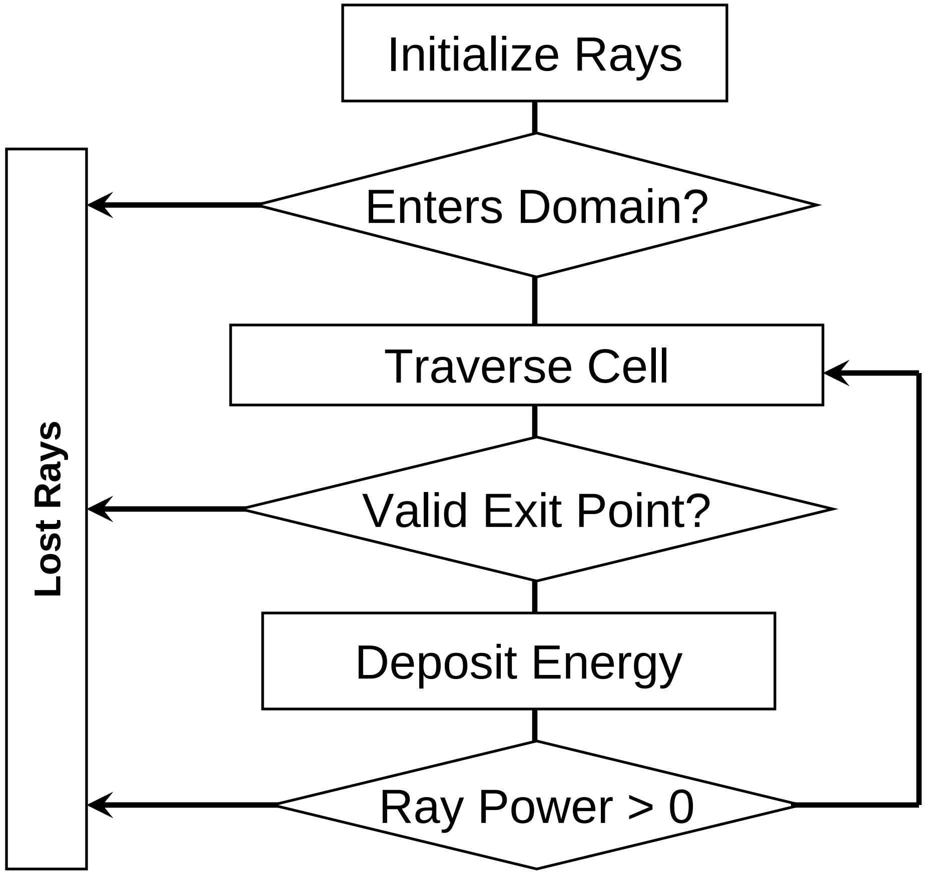
- Follow each ray through the domain
- Trajectories are, in general, quadratic due to electron density gradients
- Cell faces are DRS, intersections between the ray and surfaces involve the solution of quartic equation
- Energy Deposition is a function of ray power, electron temperature and density, and charge state
- Energy can be deposited directly or used as a source term



Right now we can trace rays through a single patch and collect the energy they deposit

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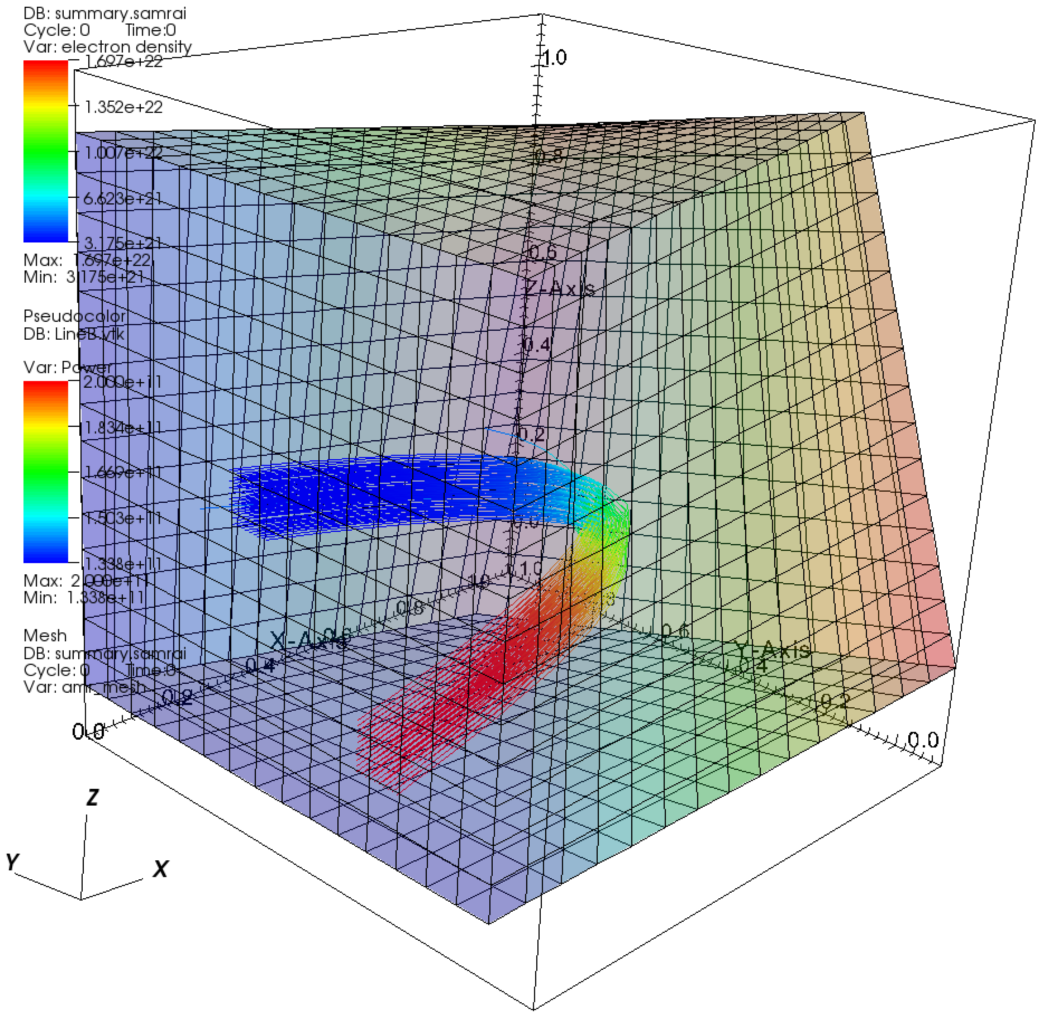

- Preliminary laser raytracing test of 100 rays with a deformed mesh (single patch) and large electron density gradient

Next steps for raytrace are AMR, parallel implementation, and use of interface reconstruction

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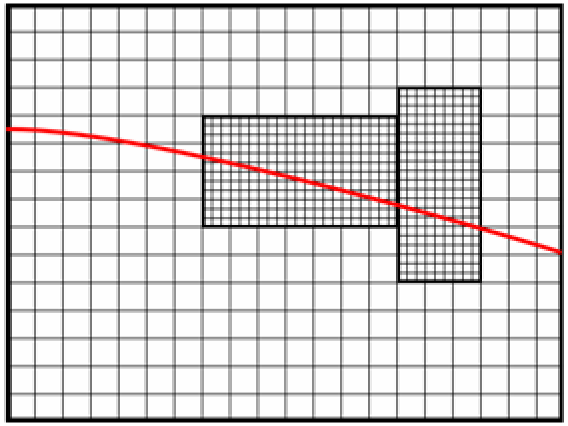
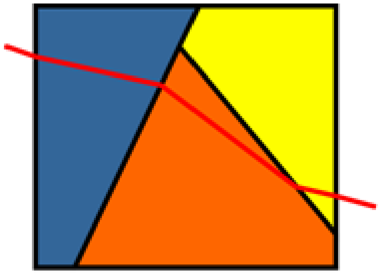
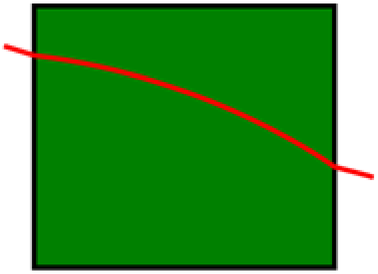


- Rays crossing patch boundaries, including refinement/coarsening boundaries, will need to be redistributed appropriately
  - Start processing with batches of rays. As these progress start subsequent batches
  - Asynchronous communication between processors to pass rays between patches/levels



Reconstructed Interfaces



Cell Average Quantities

- Interface reconstruction will be used to more accurately model laser in mixed zones
  - Rays will refract at the interfaces between constant valued component regions in mixed zones
  - Energy can be deposited in the separate component regions for accurate partitioning of laser energy

Summary

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- A complex 2D, 3D interface reconstruction scheme is implemented in NIF ALE-AMR
  - Shape function allows for non-conformal geometries
  - Final work on a few special cases is in progress
  - Application to mesh refinement step is being finalized
  - An efficient numerical implementation requires caching data

- Material interface reconstruction scheme plays a key role in target evaluations
  - Cooling ring simulations
  - Keyhole target

- Laser raytrace model in progress will allow for better energy deposition models
  - Single patch version is functional
  - Requires different parallelization model than main AMR scheme
  - Raytrace through AMR grid patches is in progress